CSC

ICT Solutions for Brilliant Minds

GPU Programming. When, Why and How?

2024

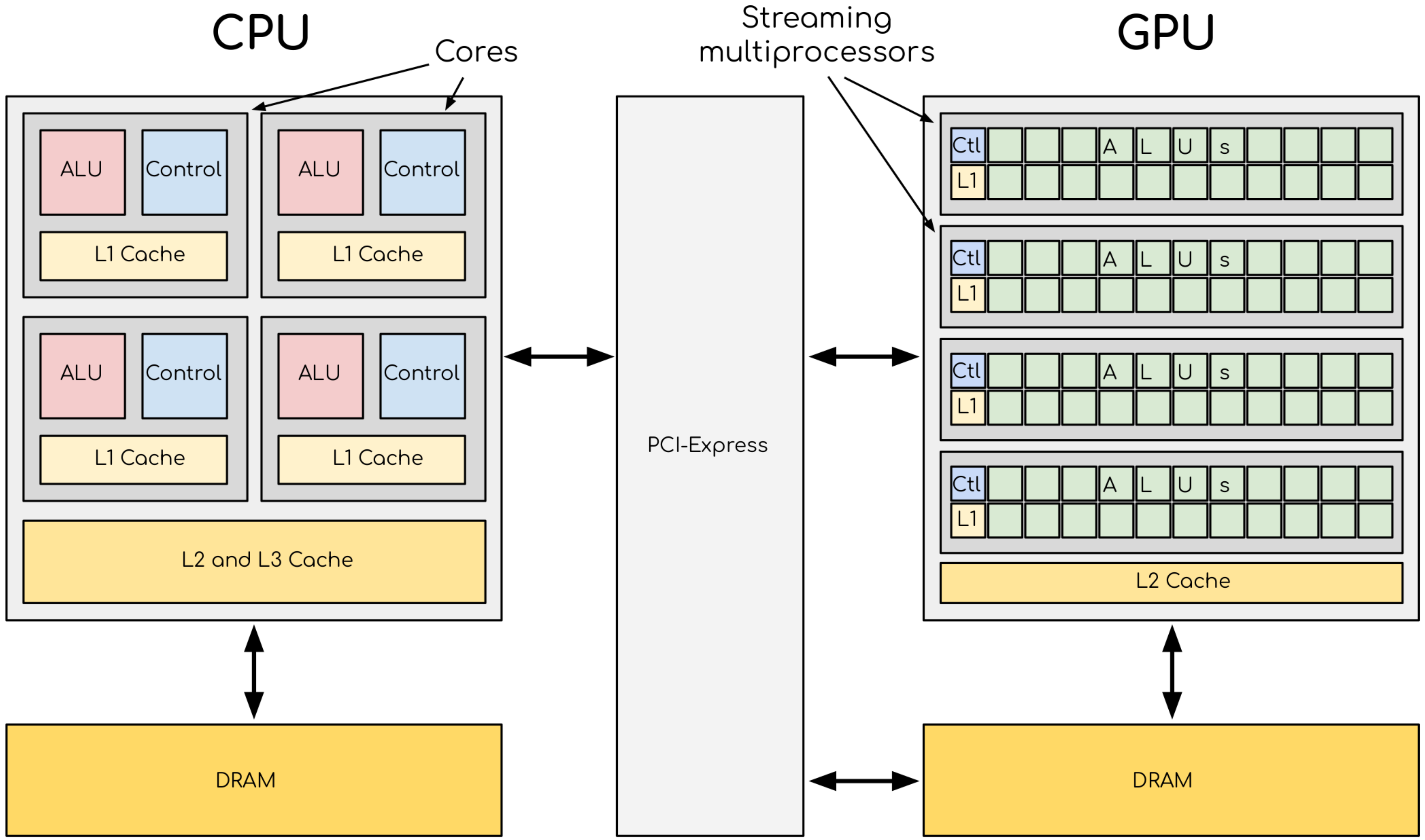
ENCCS Training

The GPU hardware and software ecosystem

Why GPUs?

- Speed: GPU computing can significantly accelerate many types of scientific workloads.
- Improved energy efficiency: GPUs can perform more calculations per watt of power consumed
- Cost-effectiveness: for certain workloads GPUs can be more cost-effective than traditional CPU-based systems.

Overview of GPU hardware



CPU (left) has complex core structure and pack several cores on a single chip. GPU cores are very simple in comparison, they also share data and control between each other.

Different design philosophies: CPU

- General purpose
- Good for serial processing
- Great for task parallelism
- Low latency per thread
- Large area dedicated cache and control
- Good for control-flow

Different design philosophies: GPU

- Highly specialized for parallelism
- Good for parallel processing
- Great for data parallelism
- High-throughput
- Hundreds of floating-point execution units
- Bad at control-flow processing

GPU Platforms

- *NVIDIA*, *AMD*, and *Intel* are the major companies which design and produce GPUs for HPC.
- GPUs are provided with their own suite **CUDA**, **ROCm**, and respectively **oneAPI**.
  - optimization, differentiation (offering unique features tailored to their devices), vendor lock-in, licensing, and royalty fees
- Cross-platform APIs such DirectCompute (only for Windows operating system), OpenCL, and SYCL.

Compute Unified Device Architecture (CUDA)

- NVIDIA's parallel computing platform.
  - Components: CUDA Toolkit & CUDA driver.
- Compilers: **nvcc**, **nvc**, **nvc++**, **nvfortran**.
  - Support GPU and multicore CPU programming (using OpenACC and OpenMP).
- CUDA API Libraries: cuBLAS, cuFFT, cuRAND, cuSPARSE.
- Debugging tools: **cuda-gdb**, **compute-sanitizer**.
- Performance analysis tools: **NVIDIA Nsight Systems**, **NVIDIA Nsight Compute**.
- Comprehensive CUDA ecosystem with extensive tools and features.

ROCm

- Open software platform for AMD accelerators.
  - Offers libraries, compilers, and development tools for AMD GPUs.
  - Supports C, C++, and Fortran languages.
  - Supports GPU and multicore CPU programming (using OpenMP and OpenCL).
- Debugging: **roc-gdb** command line tool.
- Performance analysis: **rocprof** and **roctracer** tools.
- **Heterogeneous-Computing Interface for Portability** (HIP).
  - Enables source portability for NVIDIA and AMD platforms, Intel in plan.
- Libraries: Prefixed with `roc` for AMD platforms
  - `hip`-prefixed wrappers ensure portability with no performance cost.

OneAPI

- Unified software toolkit for optimizing and deploying applications across various architectures, including CPUs, GPUs, and FPGAs.
    - Big focus on code reusability, performance, and portability.
- oneAPI **Base Toolkit**: Core set of tools and libraries for high-performance, data-centric applications. Includes SYCL support.
- oneAPI **HPC Toolkit**: additional compilers, debugging tools, MPI library, and performance analysis tool.
- Multiple programming models and languages supported: OpenMP, Classic Fortran, C++, SYCL.
- The code is portable to other OpenMP and SYCL frameworks.

Differences and similarities

- GPUs support different features, even among the same producer.
  - newer cards come with extra features and old features can become obsolete.
- Binaries have to be created targeting the specific architecture.
- **CUDA**: `-arch=sm_XY`
- **HIP** on *Nvidia*: `--gpu-architecture=sm_XY`
- **HIP** on *AMD*: `--offload-arch=gfxabc`

Terminology

NVIDIA	AMD	Intel
Streaming processor/streaming core	SIMD lane	processing element
SIMT unit	SIMD unit	Vector engine (XVE)
Streaming Multiprocessor (SMP)	Computing Unit (CU)	Xe-core / Execution unit (EU)
GPU processing clusters (GPC)	Compute Engine	Xe-slice

Summary

- GPUs allocate a larger portion of transistors to data processing rather than data caching and flow control.
- GPUs are designed to execute thousands of threads simultaneously, making them highly parallel processors. In contrast, CPUs excel at executing a smaller number of threads in parallel.
- GPU producers provide comprehensive toolkits, libraries, and compilers for developing high-performance applications that leverage the parallel processing power of GPUs. Examples include CUDA (NVIDIA), ROCm (AMD), and oneAPI (Intel).
- These platforms offer debugging tools (e.g., `cuda-gdb`, `rocgdb`) and performance analysis tools (e.g., NVIDIA Nsight Systems, NVIDIA Nsight Compute, `rocprof`, `roctracer`) to facilitate code optimization and ensure efficient utilization of GPU resources.